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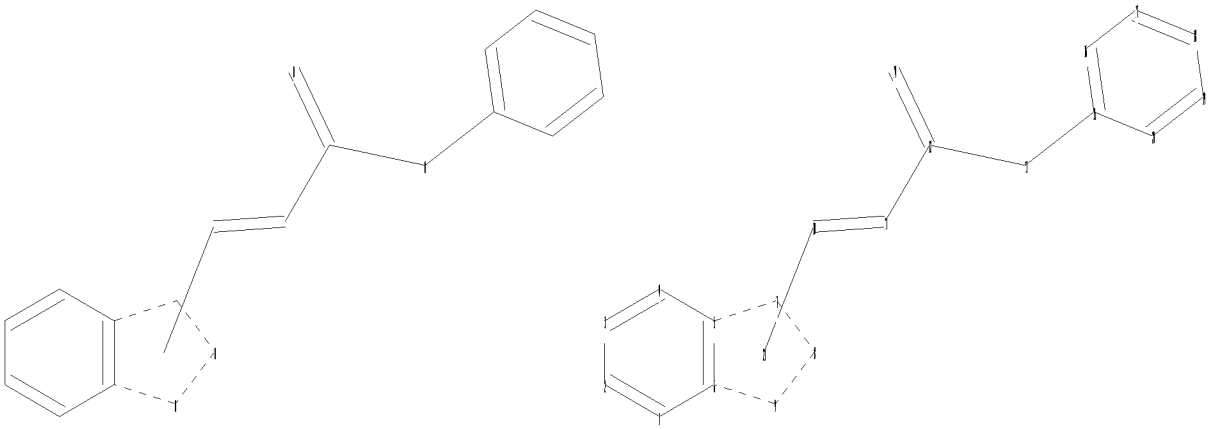
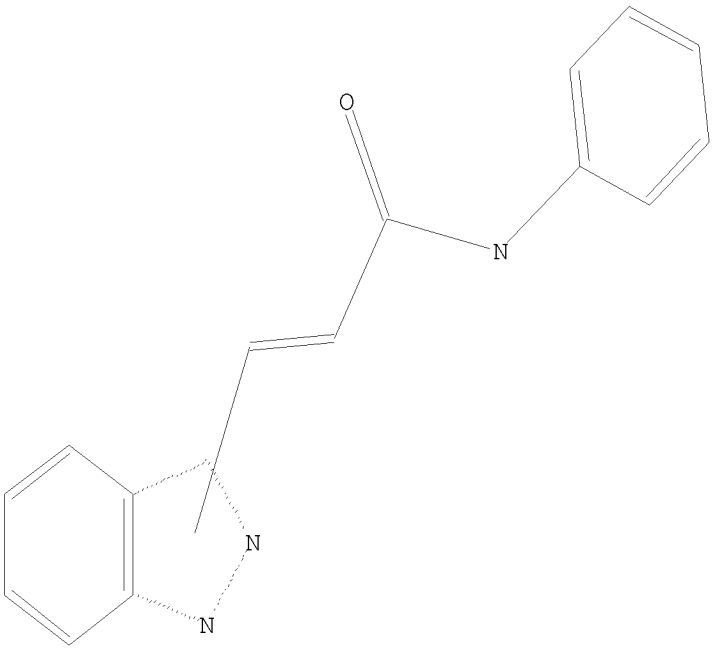


chain nodes :
10 11 12 13 14
ring nodes :
1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
10-11 11-12 12-13 12-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 15-16 15-20 16-17 17-18 18-19
19-20
exact/norm bonds :
5-7 6-9 7-8 8-9 12-13 12-14 13-15
exact bonds :
10-11 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

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=> s l5 sss sam
SAMPLE SEARCH INITIATED 11:14:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      151 TO ITERATE

100.0% PROCESSED      151 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2283 TO     3757
PROJECTED ANSWERS:               3 TO      163

L6            3 SEA SSS SAM L5

=> s l5 sss full
FULL SEARCH INITIATED 11:14:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2662 TO ITERATE

100.0% PROCESSED     2662 ITERATIONS                              37 ANSWERS
SEARCH TIME: 00.00.01

L7           37 SEA SSS FUL L5

=> file caplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
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FULL ESTIMATED COST 178.82 384.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

CA SUBSCRIBER PRICE 0.00 -3.20

FILE 'CAPLUS' ENTERED AT 11:15:09 ON 08 MAY 2008
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FILE COVERS 1907 - 8 May 2008 VOL 148 ISS 19
FILE LAST UPDATED: 7 May 2008 (20080507/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l7
L8 4 L7

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 4 ANSWERS - CONTINUE? Y/(N):y

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:120732 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 142:219278
TITLE: Preparation of indazolylacrylamides as SGK-1 inhibitors
INVENTOR(S): Drewry, David Harold; Linn, James Andrew; Veal, James Marvin
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005011681	A1	20050210	WO 2004-US23680	20040723

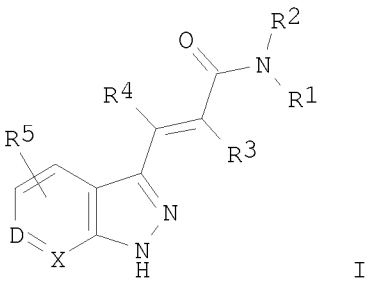
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

EP 1648448	A1	20060426	EP 2004-778961		20040723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR					
JP 2007500700	T	20070118	JP 2006-521933		20040723
US 20080058515	A1	20080306	US 2006-566040		20060126
PRIORITY APPLN. INFO.:			US 2003-490828P	P	20030729
			WO 2004-US23680	W	20040723

OTHER SOURCE(S): CASREACT 142:219278; MARPAT 142:219278

GI



I

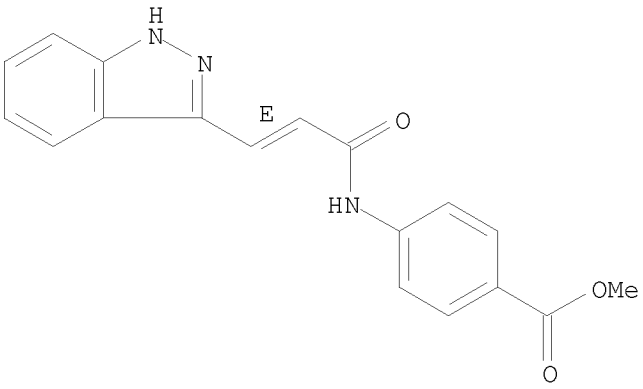
AB The title compds. I [D = CR and X = N, or D = N and X = CR, or D and X = CR (wherein R = H, halo, CN, alkyl); R1 = (Q)m(Q1)n(Q2)p (wherein Q = arylene, heteroarylene; m = 0-1; Q1 = O(CH2)q, (CH2)rC(O), SO2; n = 0-1; q = 0-4; r = 1-4; Q2 = alkyl, cycloalkyl, OH, etc.; p = 0-1); R2 = H, alkyl; NR1R2 = (un)substituted heterocyclyl, heterocyclic spiro ring system; R3, R4 = H, alkyl; R5 = H, halo, CN, OH, etc.] which are useful in the treatment of diseases mediated by inappropriate SGK-1 activity, were prepared Thus, reacting acryloyl chloride with 1,3-benzothiazol-6-amine followed by reaction of the resulting crude intermediate with 3-iodoindazole afforded I [D, X = CH; R1 = 1,3-benzothiazol-6-yl; R2-R5 = H] which showed pIC50 of > 6.0 against SGK-1. The pharmaceutical composition comprising the compound I is disclosed.

IT 842132-03-0P 842132-04-1P 842132-05-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of indazolylacrylamides as SGK-1 inhibitors)

RN 842132-03-0 CAPLUS

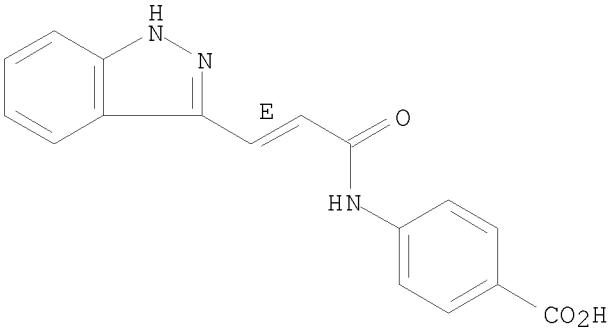
CN Benzoic acid, 4-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



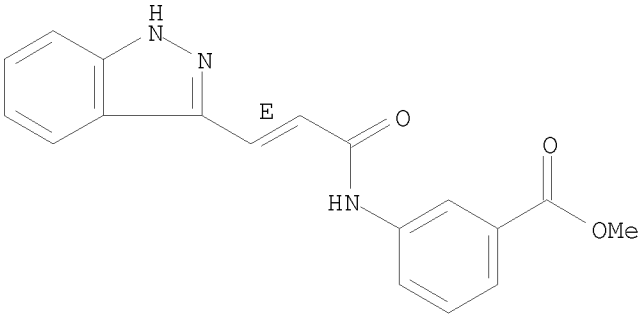
RN 842132-04-1 CAPLUS
CN Benzoic acid, 4-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-
(CA INDEX NAME)

Double bond geometry as shown.



RN 842132-05-2 CAPLUS
CN Benzoic acid, 3-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-,
methyl ester (CA INDEX NAME)

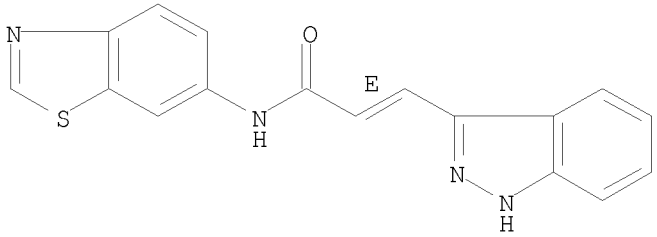
Double bond geometry as shown.



IT 842131-72-0P 842131-74-2P 842131-76-4P
842131-77-5P 842131-78-6P 842131-80-0P
842131-81-1P 842131-82-2P 842131-83-3P
842131-84-4P 842131-85-5P 842131-86-6P
842131-87-7P 842131-88-8P 842131-89-9P
842131-90-2P 842131-91-3P 842131-92-4P
842131-93-5P 842132-06-3P 842132-07-4P
842132-08-5P 842132-09-6P 842132-10-9P
842132-11-0P 842132-12-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indazolylacrylamides as SGK-1 inhibitors)

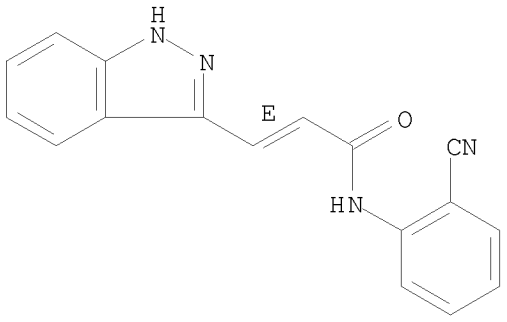
RN 842131-72-0 CAPLUS
CN 2-Propenamide, N-6-benzothiazolyl-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



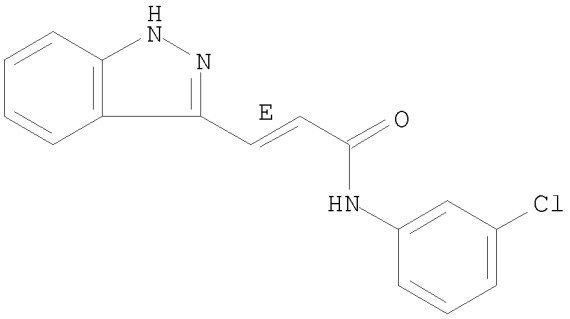
RN 842131-74-2 CAPLUS
CN 2-Propenamide, N-(2-cyanophenyl)-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



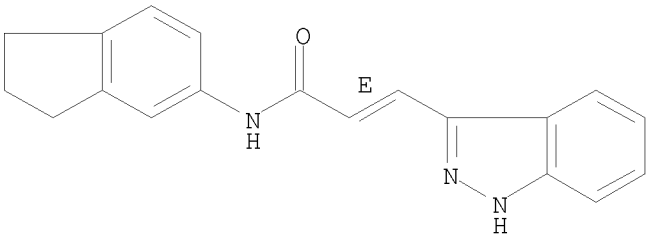
RN 842131-76-4 CAPLUS
CN 2-Propenamide, N-(3-chlorophenyl)-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



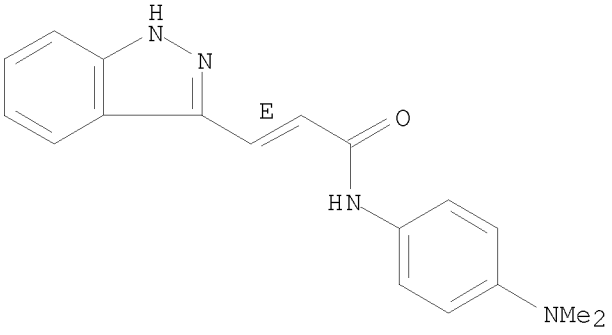
RN 842131-77-5 CAPLUS
CN 2-Propenamide, N-(2,3-dihydro-1H-inden-5-yl)-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



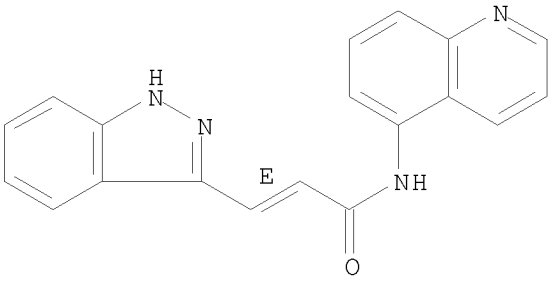
RN 842131-78-6 CAPLUS
CN 2-Propenamide, N-[4-(dimethylamino)phenyl]-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



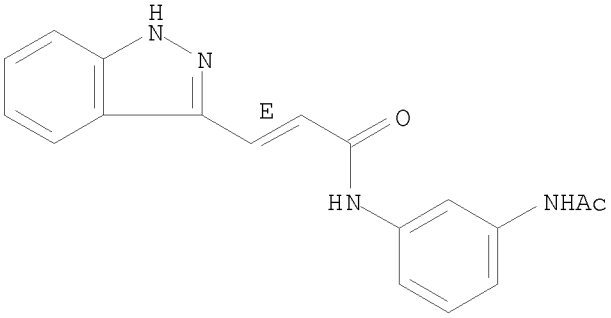
RN 842131-80-0 CAPLUS
CN 2-Propenamide, 3-(1H-indazol-3-yl)-N-5-quinolinyl-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



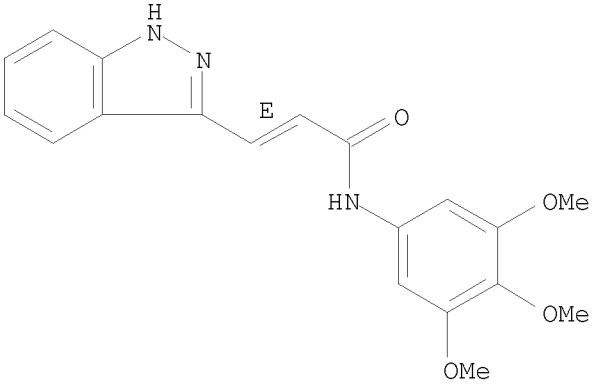
RN 842131-81-1 CAPLUS
CN 2-Propenamide, N-[3-(acetylamino)phenyl]-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



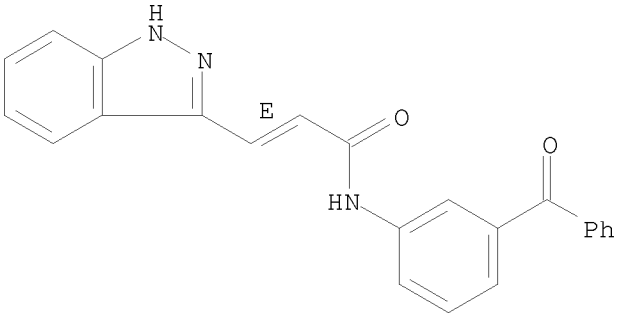
RN 842131-82-2 CAPLUS
CN 2-Propenamide, 3-(1H-indazol-3-yl)-N-(3,4,5-trimethoxyphenyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



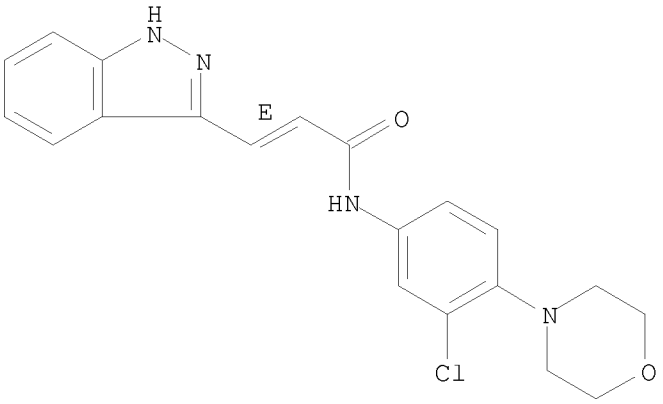
RN 842131-83-3 CAPLUS
CN 2-Propenamide, N-(3-benzoylphenyl)-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



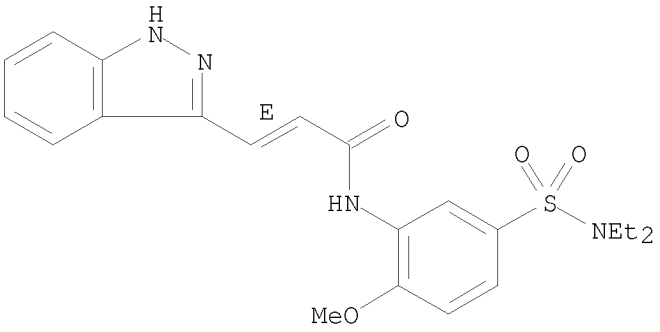
RN 842131-84-4 CAPLUS
CN 2-Propenamide, N-[3-chloro-4-(4-morpholinyl)phenyl]-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



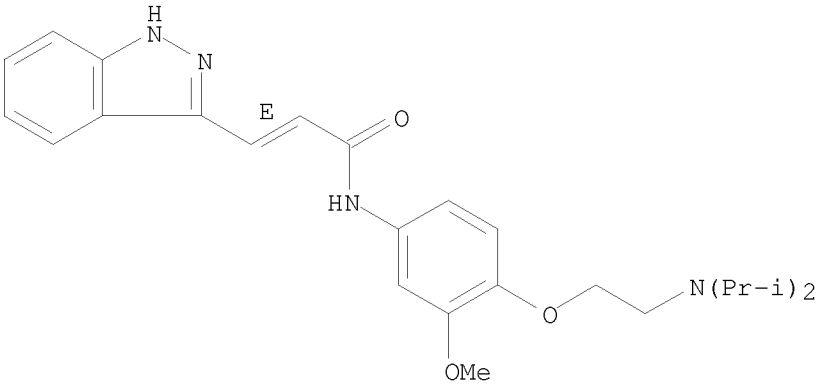
RN 842131-85-5 CAPLUS
CN 2-Propenamide, N-[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



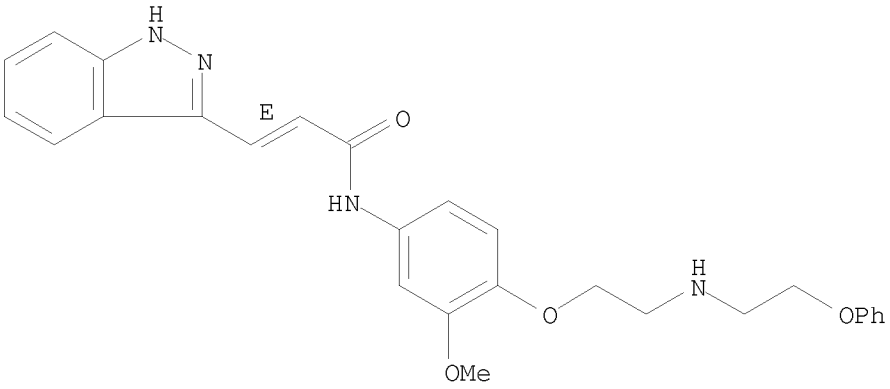
RN 842131-86-6 CAPLUS
CN 2-Propenamide, N-[4-[2-[bis(1-methylethyl)amino]ethoxy]-3-methoxyphenyl]-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



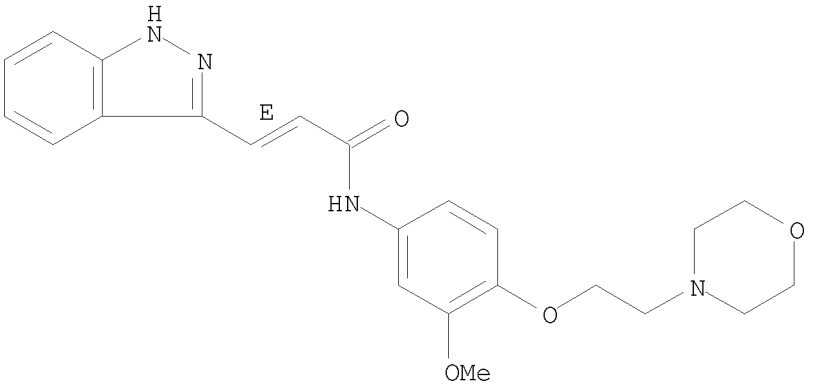
RN 842131-87-7 CAPLUS
CN 2-Propenamide, 3-(1H-indazol-3-yl)-N-[3-methoxy-4-[2-[(2-phenoxyethyl)amino]ethoxy]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



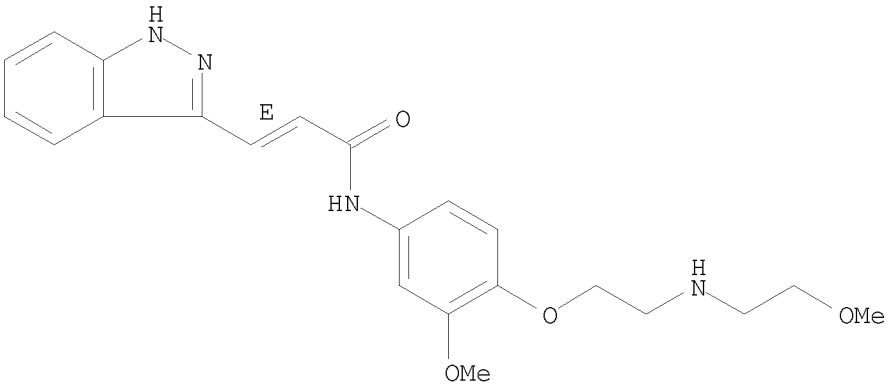
RN 842131-88-8 CAPLUS
CN 2-Propenamide, 3-(1H-indazol-3-yl)-N-[3-methoxy-4-[2-(4-morpholinyl)ethoxy]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



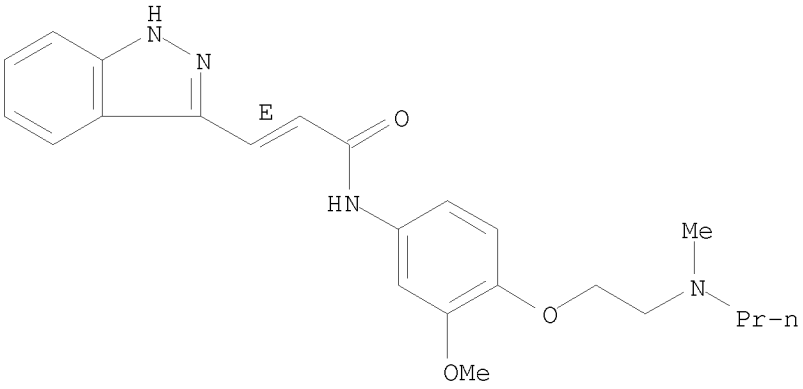
RN 842131-89-9 CAPLUS
CN 2-Propenamide, 3-(1H-indazol-3-yl)-N-[3-methoxy-4-[2-[(2-methoxyethyl)amino]ethoxy]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



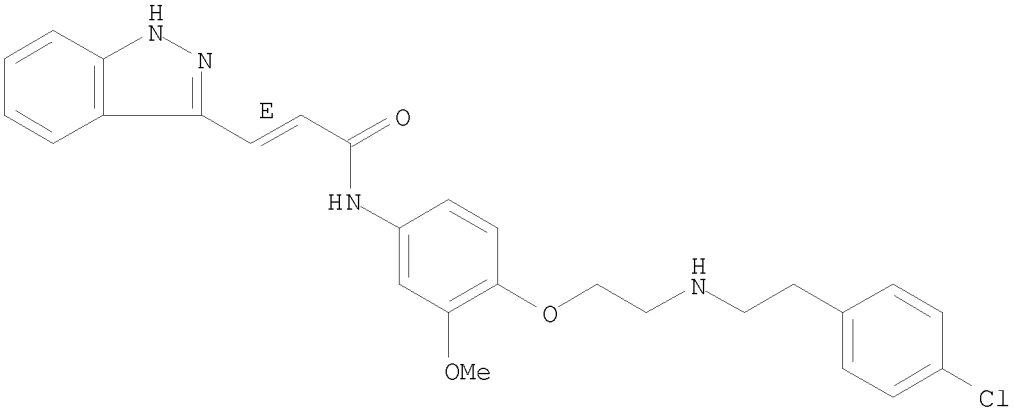
RN 842131-90-2 CAPLUS
CN 2-Propenamide, 3-(1H-indazol-3-yl)-N-[3-methoxy-4-[2-(methylpropylamino)ethoxy]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



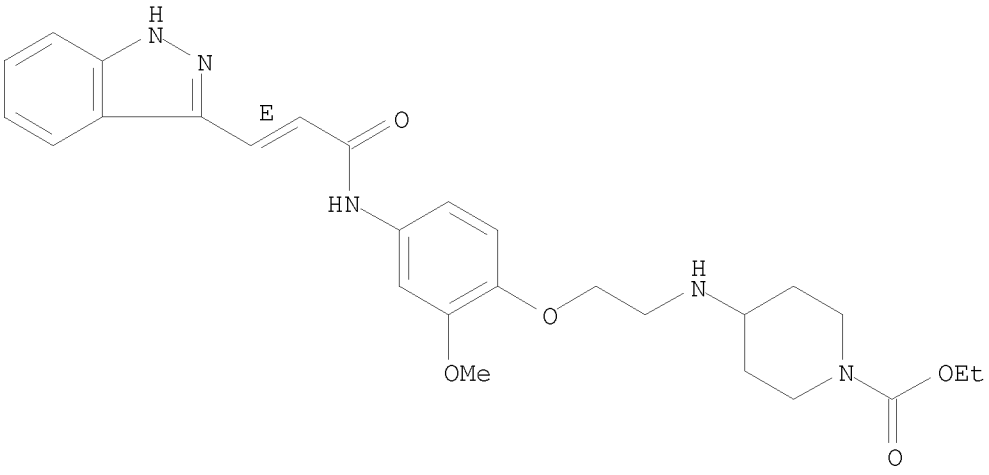
RN 842131-91-3 CAPLUS
CN 2-Propenamide, N-[4-[2-[[2-(4-chlorophenyl)ethyl]amino]ethoxy]-3-methoxyphenyl]-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



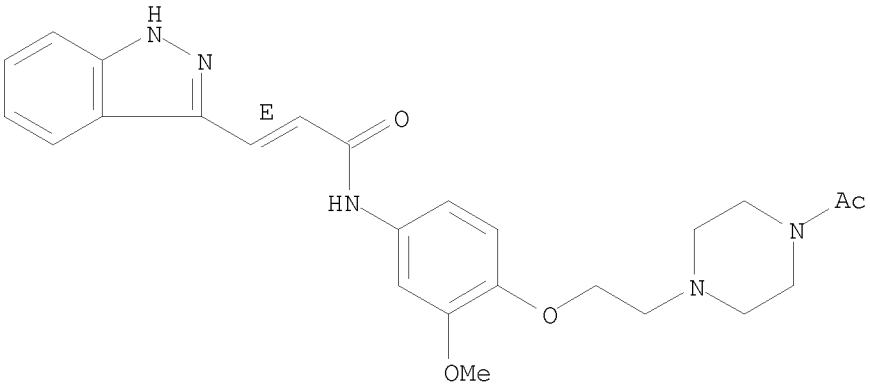
RN 842131-92-4 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[2-[4-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-2-methoxyphenoxy]ethyl]amino]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



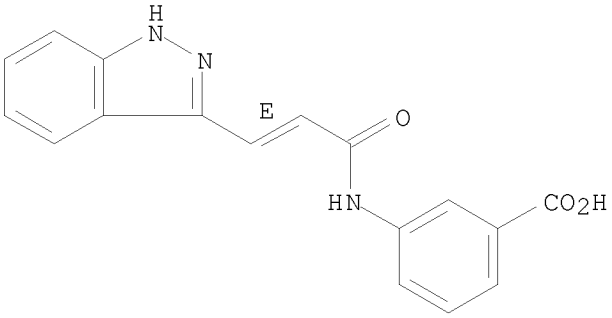
RN 842131-93-5 CAPLUS
CN 2-Propenamide, N-[4-[2-(4-acetyl-1-piperazinyl)ethoxy]-3-methoxyphenyl]-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



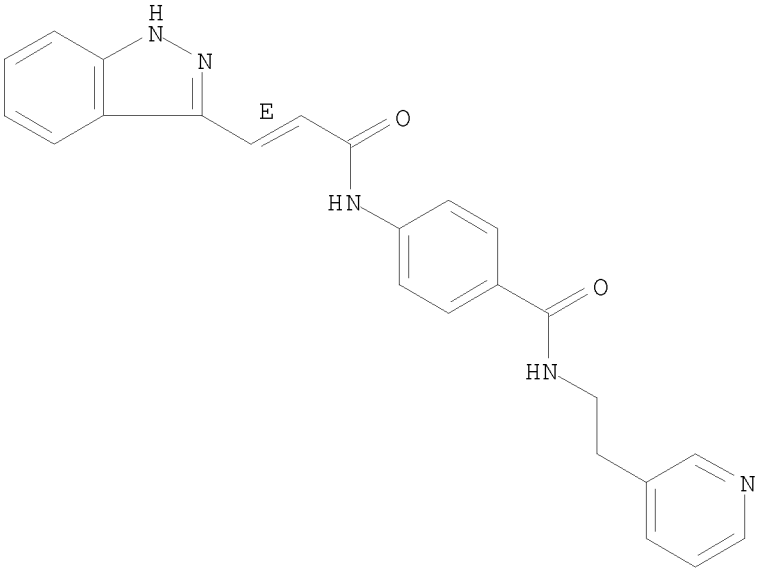
RN 842132-06-3 CAPLUS
CN Benzoic acid, 3-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-
(CA INDEX NAME)

Double bond geometry as shown.



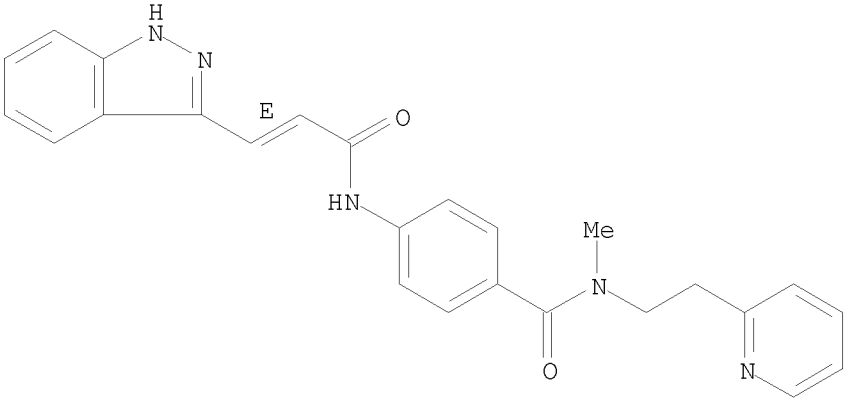
RN 842132-07-4 CAPLUS
CN Benzamide, 4-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-N-[2-(3-
pyridinyl)ethyl]- (CA INDEX NAME)

Double bond geometry as shown.



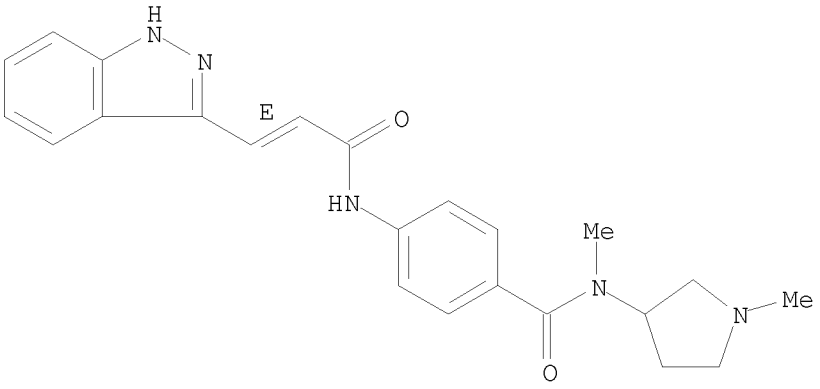
RN 842132-08-5 CAPLUS
CN Benzamide, 4-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-N-methyl-N-[2-(2-pyridinyl)ethyl]- (CA INDEX NAME)

Double bond geometry as shown.



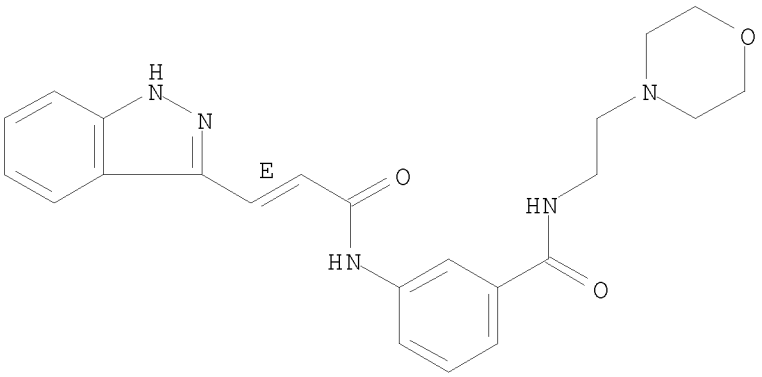
RN 842132-09-6 CAPLUS
CN Benzamide, 4-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-N-methyl-N-(1-methyl-3-pyrrolidinyl)- (CA INDEX NAME)

Double bond geometry as shown.



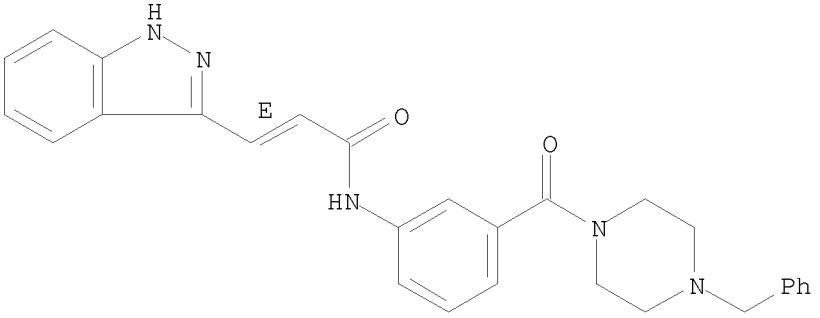
RN 842132-10-9 CAPLUS
CN Benzamide, 3-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)

Double bond geometry as shown.



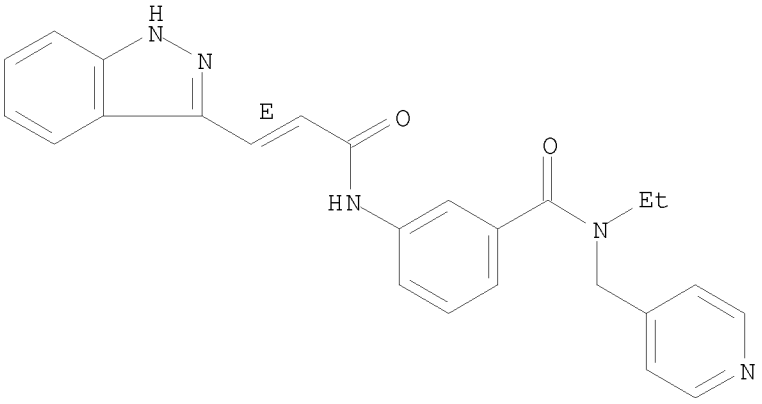
RN 842132-11-0 CAPLUS
CN 2-Propenamide, 3-(1H-indazol-3-yl)-N-[3-[[4-(phenylmethyl)-1-piperazinyl]carbonyl]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



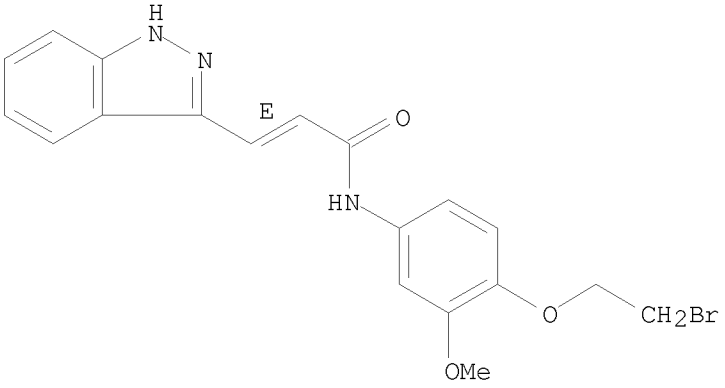
RN 842132-12-1 CAPLUS
CN Benzamide, N-ethyl-3-[[(2E)-3-(1H-indazol-3-yl)-1-oxo-2-propen-1-yl]amino]-N-(4-pyridinylmethyl)- (CA INDEX NAME)

Double bond geometry as shown.



IT 842132-16-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indazolylacrylamides as SGK-1 inhibitors)
RN 842132-16-5 CAPLUS
CN 2-Propenamide, N-[4-(2-bromoethoxy)-3-methoxyphenyl]-3-(1H-indazol-3-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



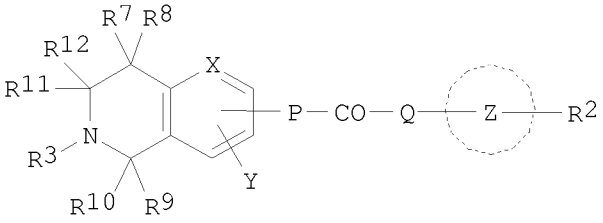
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:117027 CAPLUS <<LOGINID::20080508>>

DOCUMENT NUMBER: 132:166128
TITLE: Preparation of substituted isoquinolines as anticonvulsants
INVENTOR(S): Coulton, Steven; Harling, John David; Porter, Roderick Alan; Thompson, Mervyn
PATENT ASSIGNEE(S): Smithkline Beecham Plc, UK
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007993	A1	20000217	WO 1999-EP5583	19990803
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			GB 1998-16984 A	19980805

OTHER SOURCE(S): MARPAT 132:166128
GI



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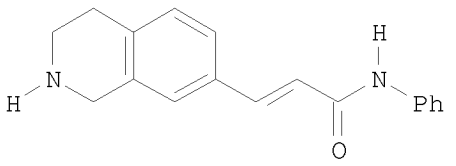


II

AB The title compds. [I; Z = a carbocyclic or heterocyclic or a fused carbocyclic or heterocyclic ring containing at least one aromatic ring; X = CH, N; Y = H, alkyl, halo; P = CH:CH and Q = NR1, or P = CH:CH and Q = NR1CH2, or P = NH and Q = CR1a:CH; R1 = H, phenylalkyl, alkyl; R1a = H, halo, phenylalkyl, alkyl; R2 = H, halo, NO2, etc.; R3 = H, phenylalkyl, alkyl, etc.; R7-R12 = H, alkyl] including tetrahydroisoquinolinyl cinnamides and acrylamides which are indicated to be useful for the treatment and/or prevention of anxiety, mania, depression, panic disorders and/or aggression, disorders associated with a subarachnoid hemorrhage or neural

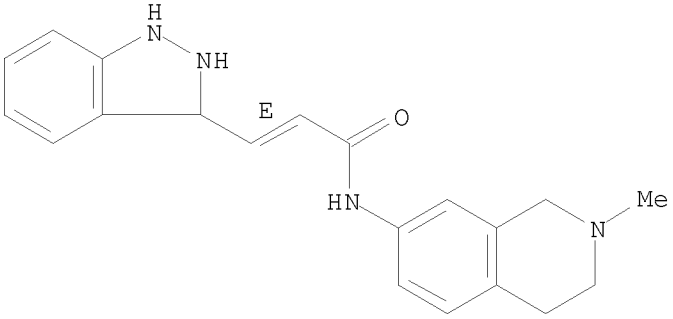
shock, the effects associated with withdrawal from substances of abuse such as cocaine, nicotine, alc. and benzodiazepines, disorders treatable and/or preventable with anti-convulsive agents, such as epilepsy including post-traumatic epilepsy, Parkinson's disease, etc., were prepared Thus, reacting (E)-7-(2-carboxyvinyl)-3,4-dihydro-1H-isoquinoline-2-carboxylic acid tert-Bu ester with aniline followed by treatment of the intermediate with trifluoroacetic acid afforded (E)-II which showed statistically significant increase (140%) in seizure threshold at 10 mg/kg p.o. in mice (MEST test).

IT 258514-53-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted isoquinolines as anticonvulsants)

RN 258514-53-3 CAPLUS

CN 2-Propenamide, 3-(2,3-dihydro-1H-indazol-3-yl)-N-(1,2,3,4-tetrahydro-2-methyl-7-isoquinolinyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:233906 CAPLUS <<LOGINID::20080508>>

DOCUMENT NUMBER: 130:267434

TITLE: Preparation of 2-cyano-3-oxo-3-benz[g]indazolepropanamides and analogs as kynurenine-3-hydroxylase inhibitors

INVENTOR(S): Pevarello, Paolo; Varasi, Mario; Amici, Raffaella; Toma, Salvatore; Speciale, Carmela

PATENT ASSIGNEE(S): Pharmacia & Upjohn S.P.A., Italy

SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

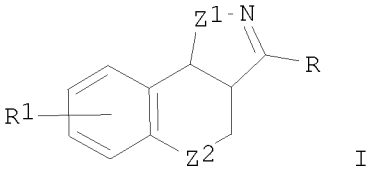
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9916753	A2	19990408	WO 1998-EP6051	19980923

WO 9916753 A3 19990520
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL, IS, JP, KE, KP, KR, LC, LK, LR, LS, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
CA 2302025 A1 19990408 CA 1998-2302025 19980923
AU 9913343 A 19990423 AU 1999-13343 19980923
EP 1019380 A2 20000719 EP 1998-956836 19980923
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
JP 2001518469 T 20011016 JP 2000-513839 19980923
PRIORITY APPLN. INFO.: GB 1997-20899 A 19971001
WO 1998-EP6051 W 19980923

OTHER SOURCE(S): MARPAT 130:267434
GI



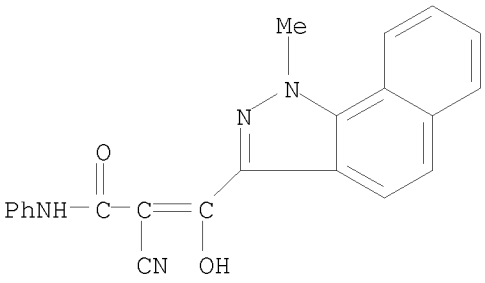
I

AB Title compds. [I; R = COCH(CN)Z(CH2)mR2; R1 = H or 1-2 of halo, alkyl, alkoxy, etc.; R2 = alkyl, (un)substituted Ph, -heterocyclyl; Z = CONH, CO, SO2; Z1 = O or NR3; R3 = alkyl, CH2Ph, pyridyl, etc.; Z2 = N, NO, CH; m = 0-6] were prepared Thus, α-tetralone was condensed with (CO2Et)2 and the product cyclocondensed with MeNHNH2 to give, after dehydrogenation, I (Z1 = MeN, Z2 = CH)(II; R = CO2Et) which was condensed with MeCN and the product condensed with PhNCO to give II [R = C(OH):CH(CN)CONHPh](III). Data for biol. activity of III Na salt were given.

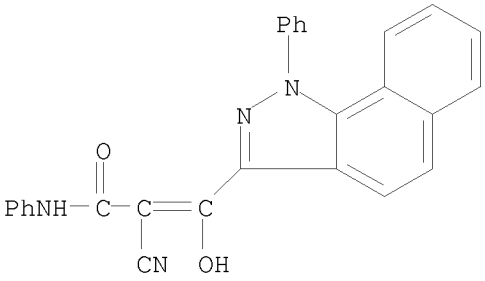
IT 222293-75-6P 222293-78-9P 222293-82-5P
222293-83-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-cyano-3-oxo-3-benz[g]indazolepropanamides and analogs as kynurenine-3-hydroxylase inhibitors)

RN 222293-75-6 CAPLUS

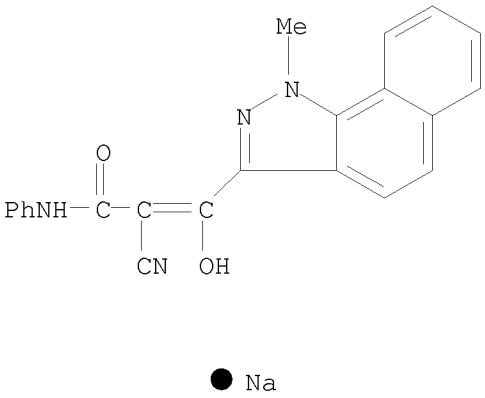
CN 2-Propenamide, 2-cyano-3-hydroxy-3-(1-methyl-1H-benz[g]indazol-3-yl)-N-phenyl- (CA INDEX NAME)



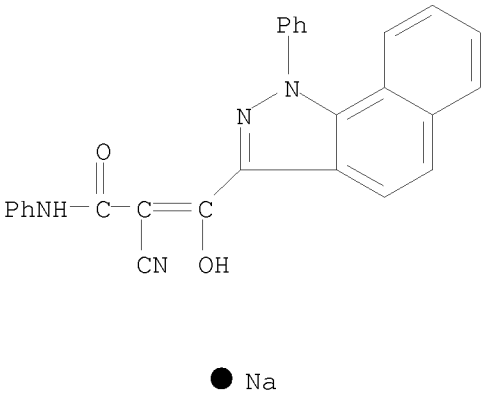
RN 222293-78-9 CAPLUS
CN 2-Propenamide, 2-cyano-3-hydroxy-N-phenyl-3-(1-phenyl-1H-benz[g]indazol-3-yl)- (CA INDEX NAME)



RN 222293-82-5 CAPLUS
CN 2-Propenamide, 2-cyano-3-hydroxy-3-(1-methyl-1H-benz[g]indazol-3-yl)-N-phenyl-, monosodium salt (9CI) (CA INDEX NAME)



RN 222293-83-6 CAPLUS
CN 2-Propenamide, 2-cyano-3-hydroxy-N-phenyl-3-(1-phenyl-1H-benz[g]indazol-3-yl)-, monosodium salt (9CI) (CA INDEX NAME)



L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:113653 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 130:168365
TITLE: Preparation of fused heterocyclic compounds as kynurenine-3-hydroxylase inhibitors
INVENTOR(S): Pevarello, Paolo; Varasi, Mario; Heidempergher, Franco; Greco, Felicita; Speciale, Carmela
PATENT ASSIGNEE(S): Pharmacia & Upjohn S.p.A., Italy
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9906375	A1	19990211	WO 1998-EP4218		19980702
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, JP, KE, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
CA 2296606	A1	19990211	CA 1998-2296606		19980702
AU 9887317	A	19990222	AU 1998-87317		19980702
EP 1001941	A1	20000524	EP 1998-938689		19980702
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
JP 2001512107	T	20010821	JP 2000-505134		19980702
PRIORITY APPLN. INFO.:			GB 1997-16101	A	19970730
			WO 1998-EP4218	W	19980702

OTHER SOURCE(S): MARPAT 130:168365
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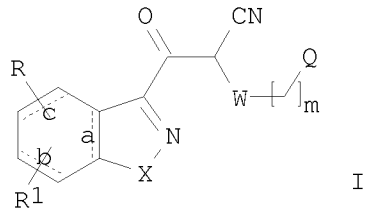

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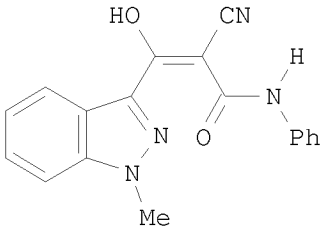


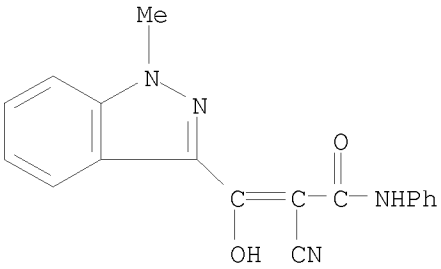
II

AB The title compds. [I; a, b, c = all single bonds; or a, b, c = all double bonds; or a = double bond and b, c = single bonds; m = 0-6; W = CONH, SO2, CO; X = O, S, NR2 (wherein R2 = H, C1-6 alkyl, PhCH2, etc.); R, R1 = H, halo, OH, etc.; Q = C1-14 alkyl, (un)substituted Ph ring or unsatd. pentat. heteromonocyclic ring containing two or three heteroatoms chosen independently from O, S and N], useful as kynurenine-3-hydroxylase inhibitors, were prepared and formulated. Thus, treatment of 2-cyano-3-(1-methyl-1H-indazol-3-yl)-3-oxo-N-phenylpropanamide (preparation given) with 0.1 N NaOH in EtOH afforded acrylamide II as sodium salt which showed IC50 of 1.1 μM against KYN-3-OH.

IT 220487-67-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fused heterocyclic compds. as kynurenine-3-hydroxylase inhibitors)

RN 220487-67-2 CAPLUS

CN 2-Propenamide, 2-cyano-3-hydroxy-3-(1-methyl-1H-indazol-3-yl)-N-phenyl-, monosodium salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      24.68     409.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                      -3.20      -6.40

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STRUCTURE FILE UPDATES:    7 MAY 2008  HIGHEST RN 1019993-29-3
DICTIONARY FILE UPDATES:   7 MAY 2008  HIGHEST RN 1019993-29-3

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http://www.cas.org/support/stngen/stndoc/properties.html

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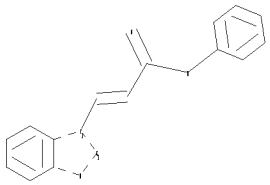

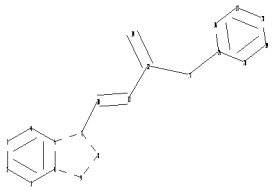

chain nodes :
10 11 12 13 14
ring nodes :
1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
7-10 10-11 11-12 12-13 12-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 15-16 15-20 16-17 17-18 18-19
19-20
exact/norm bonds :
5-7 6-9 7-8 7-10 8-9 10-11 11-12 12-13 12-14 13-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20

G1:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom

L9 STRUCTURE UPLOADED

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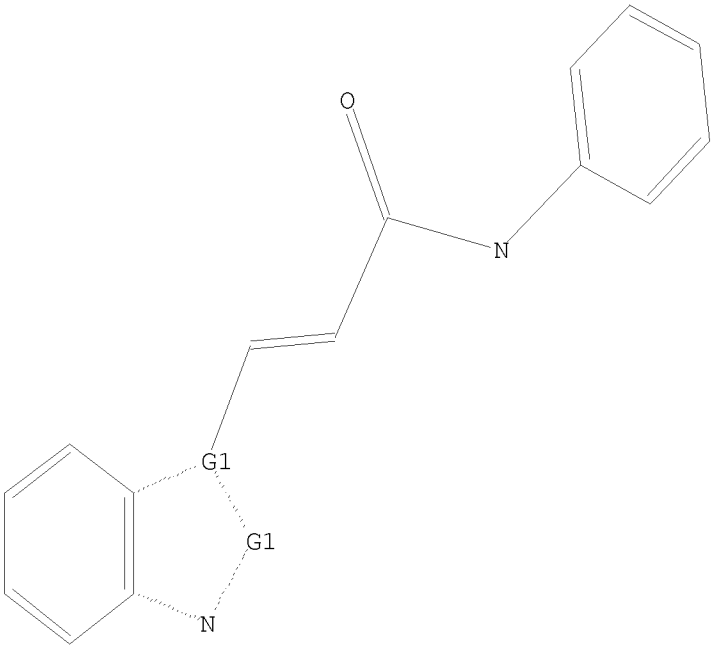
L9 HAS NO ANSWERS
L9 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 1563 TO ITERATE

100.0% PROCESSED 1563 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 28889 TO 33631
PROJECTED ANSWERS: 3009 TO 4671

L10 50 SEA SSS SAM L9

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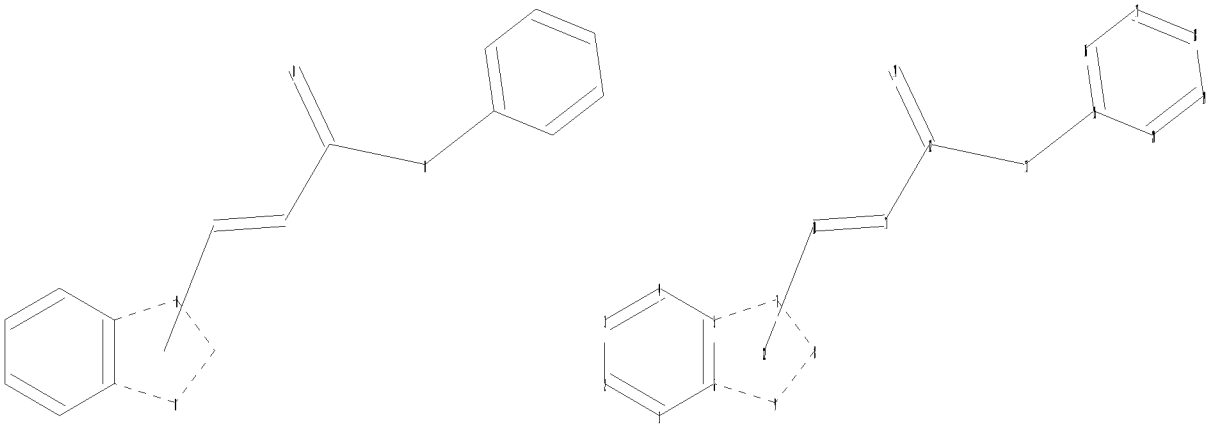

chain nodes :
10 11 12 13 14
ring nodes :
1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
10-11 11-12 12-13 12-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 15-16 15-20 16-17 17-18 18-19
19-20
exact/norm bonds :
5-7 6-9 7-8 8-9 12-13 12-14 13-15
exact bonds :
10-11 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 22:CLASS

L11 STRUCTURE UPLOADED

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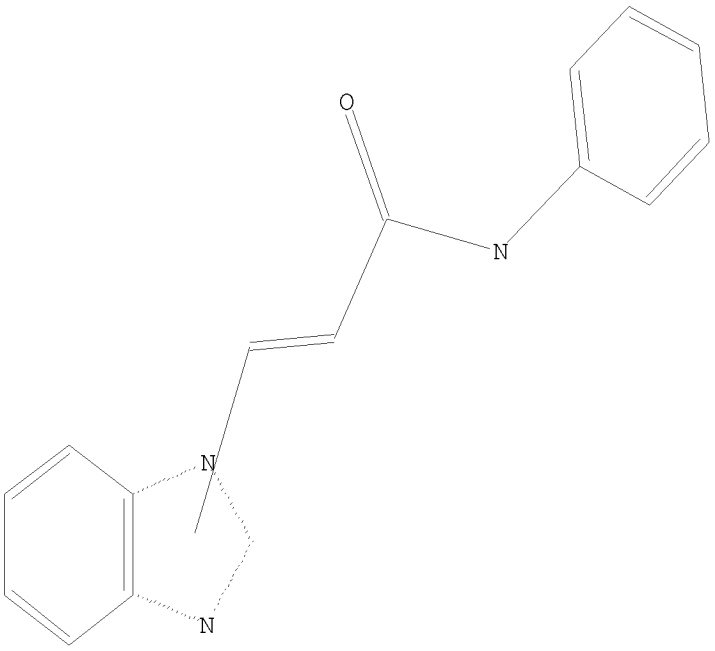
L11 HAS NO ANSWERS
L11 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -      224 TO ITERATE

100.0% PROCESSED      224 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         3583 TO     5377
PROJECTED ANSWERS:               3 TO      163

L12           3 SEA SSS SAM L11

=> s l11 sss full
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FULL SCREEN SEARCH COMPLETED -     4234 TO ITERATE

100.0% PROCESSED     4234 ITERATIONS                               38 ANSWERS
SEARCH TIME: 00.00.01

L13          38 SEA SSS FUL L11

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COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
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FILE LAST UPDATED: 7 May 2008 (20080507/ED)

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=> s l13
L14 8 L13

=> d ibib abs hitstr 1-
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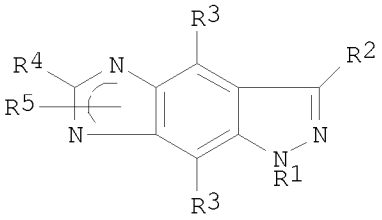
L14 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:588231 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 141:140440
TITLE: Preparation of indazoles and their use as anti-inflammatory, antirheumatic, and antiarthritic agents
INVENTOR(S): Konno, Yasuo; Ono, Tomoyasu; Kitagawa, Kazuhiro; Inoue, Shinichi; Tanaka, Katsuhisa; Yamada, Shozo; Asao, Tetsuji
PATENT ASSIGNEE(S): Taiho Pharamceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 54 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004203804	A	20040722	JP 2002-376012	20021226

PRIORITY APPLN. INFO.: JP 2002-376012 20021226
OTHER SOURCE(S): MARPAT 141:140440
GI



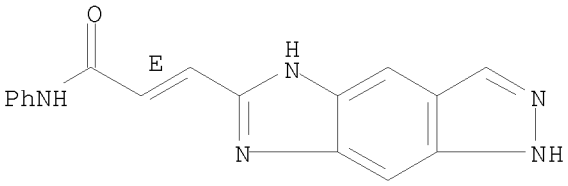
I

AB Title agents contain indazoles I [R1 = H, [(mono- or di-lower alkyl)amino-substituted] lower alkyl, acyl, lower alkoxycarbonyl, lower alkyl- or aryl-substituted SO2; R2 = H, lower alkyl(oxy); R3 = H, halo; R4 = H, (un)substituted cycloalkyl, (un)substituted aryl, (un)substituted heterocyclyl, (un)substituted NH2, acyl, etc.; R5 = H, protecting group] or their pharmacol. acceptable salts as active ingredients. Thus, cyclocondensation of 5,6-diaminoindazole with PhCHO in AcNMe2 gave 90% I (R1-R3 = R5 = H, R4 = Ph), which at 300 mg/kg p.o. inhibited type II-collagen-induced arthritis by 96.7% in mice.

IT 724766-89-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolobenzimidazoles as anti-inflammatory, antirheumatic, and antiarthritic agents)

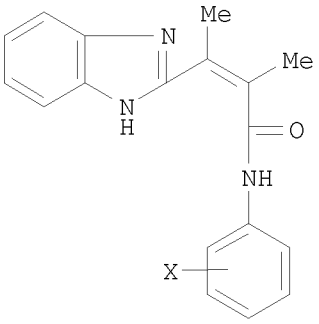
RN 724766-89-6 CAPLUS
CN 2-Propenamide, 3-(1,7-dihydroimidazo[4,5-f]indazol-6-yl)-N-phenyl-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

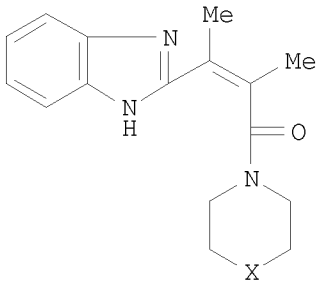


L14 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:299968 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 133:150502
TITLE: Synthesis and SAR of benzimdazole anthelmintics
AUTHOR(S): Gaur, N. M.; Patil, S. V.; Mourya, V. K.; Wagh, S. B.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, College of Pharmacy, Nashik, 420 002, India

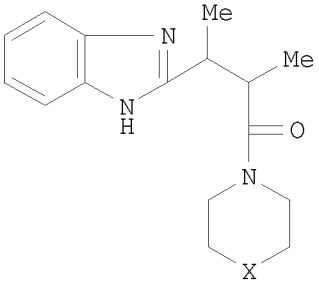
SOURCE: Indian Journal of Heterocyclic Chemistry (2000), 9(3), 227-230
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Prof. R. S. Varma
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



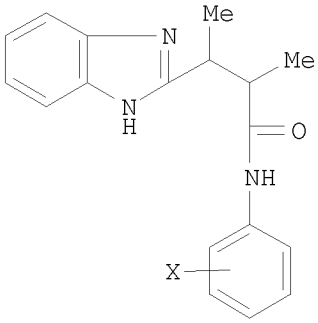
I



II



III



IV

AB β-Benzimidazolyl-α-Me crotonic acid anilides I (X = H, 3-Cl, 4-Cl, 4-Me, 4-MeO), β-benzimidazolyl α-Me crotonic acid amides II (X = O, CH2, NMe), β-benzimidazolyl Me butyramides III, and β-benzimidazolyl α-Me butyranilides IV were synthesized and tested for anthelmintic activity. It was found that the m-chloro derivative I (X = 3-Cl) showed maximum activity while p-methoxy derivative showed min. activity. A correlation of Hammett substituent constant and activity is given.

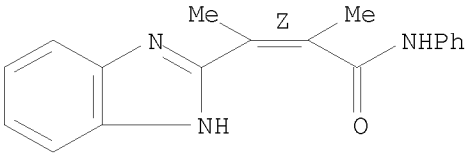
IT 286930-50-5P 286930-51-6P 286930-52-7P
286930-53-8P 286930-54-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, anthelmintic activity, structure-activity relationship, and Hammett substituent constant of benzimidazoles)

RN 286930-50-5 CAPLUS

CN 2-Butenamide, 3-(1H-benzimidazol-2-yl)-2-methyl-N-phenyl-, (2Z)- (CA

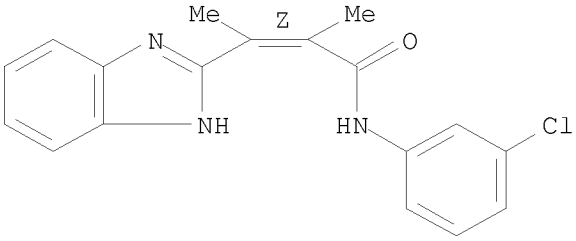
INDEX NAME)

Double bond geometry as shown.



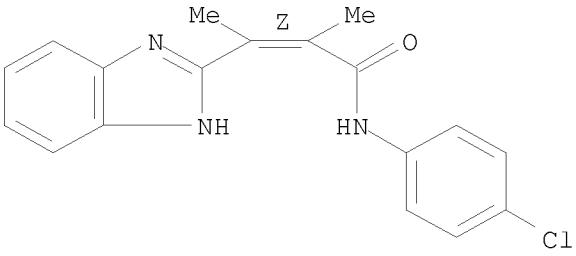
RN 286930-51-6 CAPLUS
CN 2-Butenamide, 3-(1H-benzimidazol-2-yl)-N-(3-chlorophenyl)-2-methyl-, (2Z)-
(CA INDEX NAME)

Double bond geometry as shown.



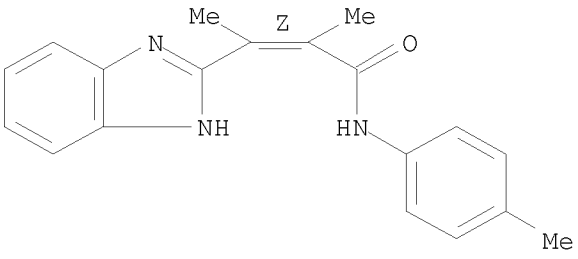
RN 286930-52-7 CAPLUS
CN 2-Butenamide, 3-(1H-benzimidazol-2-yl)-N-(4-chlorophenyl)-2-methyl-, (2Z)-
(CA INDEX NAME)

Double bond geometry as shown.



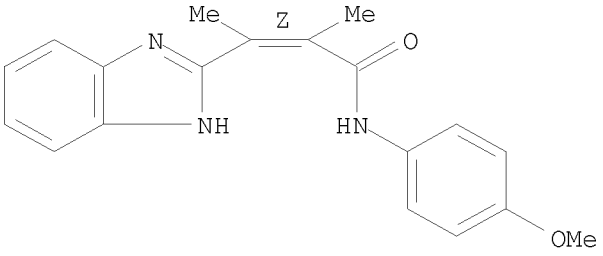
RN 286930-53-8 CAPLUS
CN 2-Butenamide, 3-(1H-benzimidazol-2-yl)-2-methyl-N-(4-methylphenyl)-, (2Z)-
(CA INDEX NAME)

Double bond geometry as shown.



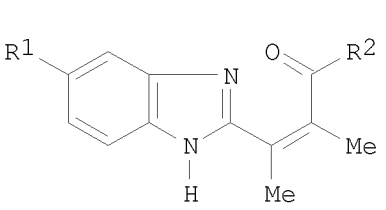
RN 286930-54-9 CAPLUS
CN 2-Butenamide, 3-(1H-benzimidazol-2-yl)-N-(4-methoxyphenyl)-2-methyl-, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

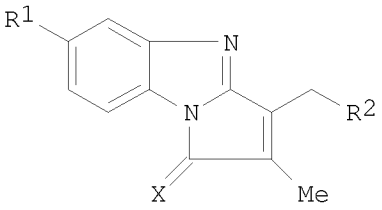


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:467095 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 131:228686
TITLE: Synthesis and novel reactions of 2,3-dimethyl-1H-pyrrolo[1,2-a]-benzimidazol-1-one with secondary amines and N-bromosuccinimide
AUTHOR(S): Shetgiri, N. P.; Kokitkar, S. V.
CORPORATE SOURCE: Department of Chemistry, The Institute of Science, Mumbai, 400 032, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1999), 38B(3), 312-316
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:228686
GI



I

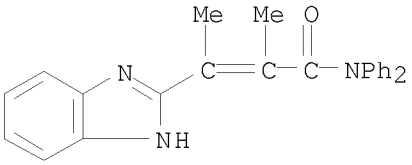


II

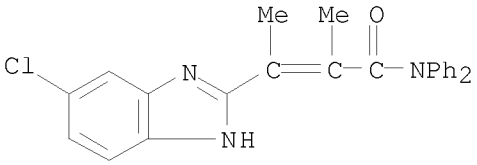
AB N,N-Disubstituted-β-(2-benzimidazolyl)-α,β-dimethylacrylamides I (R1 = H, Cl; R2 = morpholine, piperidine, etc.), 2-bromomethyl-3-methyl-1H-pyrrolo[1,2a]benzimidazol-1-one II (R1 = H; R2 = Br; X = O) and 2,3-dimethyl-1H-pyrrolo[1,2a]benzimidazole-1-thione II (R1 = R2 = H; X = S) have been synthesized from 2,3-dimethyl-1H-pyrrolo[1,2a]benzimidazol-1-one II (R1 = H, Cl; R2 = H; X = O). Compds. I have been synthesized via two different routes and screened for their antimicrobial and anthelmintic activities.

IT 243843-18-7P 243843-25-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of dimethylpyrrolobenzimidazolone and conversion to benzimidazolyldimethylacrylamides, bromomethylmethylpyrrolobenzimidazolone, and dimethylpyrrolobenzimidazolethione)

RN 243843-18-7 CAPLUS
CN 2-Butenamide, 3-(1H-benzimidazol-2-yl)-2-methyl-N,N-diphenyl- (CA INDEX NAME)

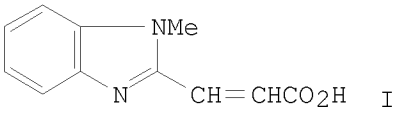


RN 243843-25-6 CAPLUS
CN 2-Butenamide, 3-(5-chloro-1H-benzimidazol-2-yl)-2-methyl-N,N-diphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

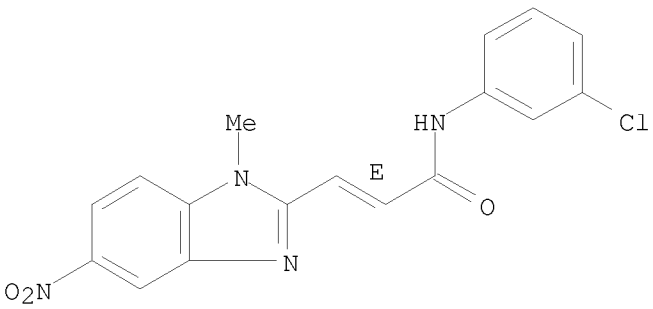
L14 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:146669 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 92:146669
ORIGINAL REFERENCE NO.: 92:23837a,23840a
TITLE: Synthesis of 3-(1-methyl-5-nitro-2-benzimidazolyl)acrylic acid derivatives as expected antischistosomal agents
AUTHOR(S): Omar, Nabil M.; Farag, Hassan H.; Omar, Farghaly A.
CORPORATE SOURCE: Fac. Pharm., Univ. Assiut, Assiut, Egypt
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1979), 34B(10), 1427-30
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 92:146669
GI



I

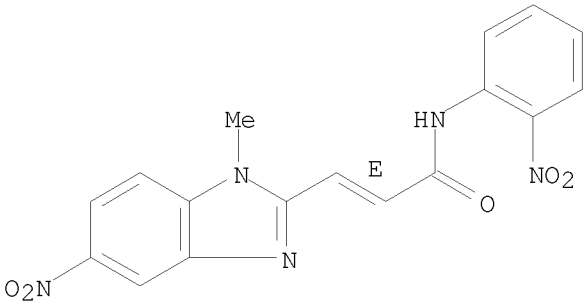
AB Several ester and amide derivs. of 3-(1-methyl-5-nitro-2-benzimidazolyl)acrylic acid (I) prepared for testing as potential antischistosomal agents. I was prepared from 1-methyl-5-nitro-2-benzimidazolecarboxaldehyde and CH2(CO2H)2. N-Ethoxycarbonyl-2-ethoxydihydroquinoline was used as the coupling agent for the esterifications and amidations.
IT 73237-63-5P 73237-64-6P 73282-60-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 73237-63-5 CAPLUS
CN 2-Propenamide, N-(3-chlorophenyl)-3-(1-methyl-5-nitro-1H-benzimidazol-2-yl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



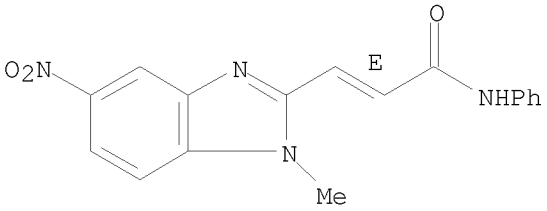
RN 73237-64-6 CAPLUS
CN 2-Propenamide, 3-(1-methyl-5-nitro-1H-benzimidazol-2-yl)-N-(2-nitrophenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



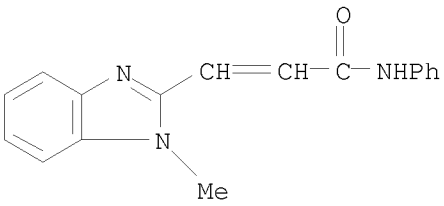
RN 73282-60-7 CAPLUS
CN 2-Propenamide, 3-(1-methyl-5-nitro-1H-benzimidazol-2-yl)-N-phenyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

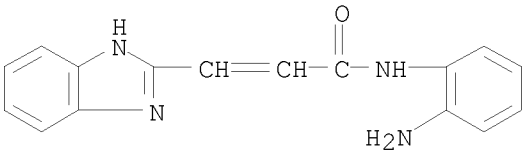


L14 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:76369 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 74:76369
ORIGINAL REFERENCE NO.: 74:12395a,12398a
TITLE: Benzimidazole derivatives. XXV. Synthesis of 3-(1-methyl-2-benzimidazolyl)acrylic acid and its derivatives
AUTHOR(S): Popov, I. I.; Simonov, A. M.; Kolodyazhnaya, S. N.
CORPORATE SOURCE: Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1970), (11), 1566-8
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Treatment of I with Cl3CCHO over ZnCl2 and then with NaOH afforded II (X = OH), which gave II (X = OR) with SOCl2 followed by ROH (R = Me, Et). II (X = OR) were also prepared by oxidizing I with SeO2, followed by treatment with Ph3P:CHCO2R. II (X = NHPh, NEt2, piperidino) were prepared from II (X

= Cl·HCl) and the corresponding amines.
IT 30780-03-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30780-03-1 CAPLUS
CN 2-Benzimidazoleacrylanilide, 1-methyl- (8CI) (CA INDEX NAME)

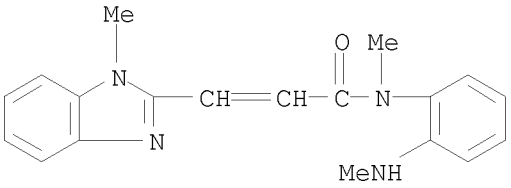


L14 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:512864 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 71:112864
ORIGINAL REFERENCE NO.: 71:21003a,21006a
TITLE: Fluorescent alkylating agents. 1-(β-chloroethyl)bisbenzimidazoles
AUTHOR(S): Tsou, Kwan Chung; Rabiger, Dorothy J.; Sobel, Barbara
CORPORATE SOURCE: Sch. of Med., Univ. of Pennsylvania, Philadelphia, PA, USA
SOURCE: Journal of Medicinal Chemistry (1969), 12(5), 818-22
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cis- and trans-1-(β-Chloroethyl)bisbenzimidazoles (I) (R = H or Me, R1 = H or Me) have been synthesized as fluorescent alkylating agents. Preliminary in vivo study with HeLa cells shows that such compounds can be useful to demonstrate the intranuclear alkylation in dividing cells.
IT 24156-52-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24156-52-3 CAPLUS
CN 2-Benzimidazoleacrylanilide, 2'-amino-, dihydrochloride (8CI) (CA INDEX NAME)



●2 HCl

L14 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:454940 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 59:54940
ORIGINAL REFERENCE NO.: 59:10024d-h
TITLE: Benzimidazole derivatives. XIII. Transformations of 2-formyl-1-methylbenzimidazole
AUTHOR(S): Dalgatov, D. D.; Simonov, A. M.
CORPORATE SOURCE: State Univ., Rostov-on-Don
SOURCE: Zhurnal Obshchei Khimii (1963), 33(3), 1007-10
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 55, 16520f; 58, 13936f. Heating 1-methyl-2-hydroxymethylbenzimidazole in 2N H_2SO_4 in the presence of $AgNO_3$ to 70° and treating the solution gradually with $K_2S_2O_8$ gave after filtration and neutralization, followed by extraction with $CHCl_3$, 1-methyl-2-formylbenzimidazole (I), m 110°; a more satisfactory preparation in 50% yield was secured by oxidation of 1,2-dimethylbenzimidazole with SeO_2 at 95° in dry dioxane. Heating 2-hydroxymethylbenzimidazole with Leueotrope O in aqueous NaOH 2 hrs. gave after removal of $PhNMe_2$ with steam 1-benzyl-2-hydroxymethylbenzimidazole, m. 186.5-7°. I and AcPh in the presence of 2% aqueous NaOH rapidly gave 83% 2-(2-benzoylvinyl)-1-methylbenzimidazole (II), m. 154-5°, which gave an orange solution in H_2SO_4 (2,4-dinitrophenylhydrazone m. 262°). This was brominated in CCl_4 to γ-(1-methyl-2-benzimidazolyl)-β,γ-dibromopropiophenone, m. 134°. II and MeI in EtOH 2 hrs. gave II methiodide, m. 236°, which with aqueous KOH 1 hr. gave yellow N-β-benzoylacrylyl-N,N'-dimethyl-o-phenylenediamine, m. 156.5°. I and AcPh in EtOH treated gradually with 20% aqueous KOH, heated briefly at 100°, and kept 2 hrs. gave colorless 1-methyl-2-bis(phenacylmethyl)benzimidazole (II), m. 184°. Similarly were prepared: yellow 2-(β-pbromobenzoylvinyl)-1-methylbenzimidazole, m. 159 60°, and colorless 1-methyl-2-bis(p-bromophenacylmethyl)benzimidazole, m. 186.5-87°. I and cyclohexanone in MeOH in the presence of 10% KOH 0.5 hr. at reflux gave yellow 2-(1-methyl-2-benzimidazolylmethylene)eyclohexanone, m. 237°. I and 1,2-dimethylbenzimidazole-MeI in MeOH-piperidine 4 hrs. gave yellow 1,2-bis(1-methyl-2-benzimidazolyl)ethylene-MeI (III), decomposed 273°, which with aqueous alc. KOH 1 hr. gave yellow N-[β-(1-methyl-2-benzimidazolyl)acryloyl]-N,N'-dimethyl-o-phenylenediamine, m. 186°. 1,2-Dimethylbenzimidazole with excess EtI gave the monoethiodide, m. 188-90°. 1,2-bis(1-methyl-2-benzimidazolyl)ethene-EtI, yellow, m. 232-3°.
IT 97078-58-5P, Acrylanilide, N-methyl-2'-(methylamino)-3-(1-methyl-2-benzimidazolyl-
RL: PREP (Preparation)
(preparation of)
RN 97078-58-5 CAPLUS
CN 2-Benzimidazoleacrylanilide, N,1-dimethyl-2'-(methylamino)- (7CI) (CA INDEX NAME)



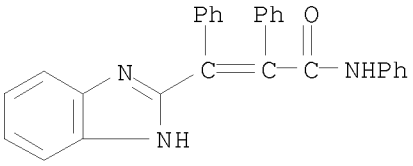
L14 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1923:19661 CAPLUS <<LOGINID::20080508>>
DOCUMENT NUMBER: 17:19661
ORIGINAL REFERENCE NO.: 17:3027b-i
TITLE: Action of o-phenylenediamine upon the anhydrides of diphenyhnaleic, homophthalic and diphenic acids
AUTHOR(S): Bistrzycki, A.; Fassler, Karl
SOURCE: Helvetica Chimica Acta (1923), 6, 519-35
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Diphenylmaleic anhydride and o-C6H4(NH2)2 in boiling EtOH give an 85-905 yield of N-[2''-aminophenyl]diphenylmaleic imide (diphenylmaleic-2''-aminoanil), orange-yellow, decomps. 207-8°. In spite of the free NH2 group, it is insol. in HCl. Ac derivative, yellow, m. 224°. Heated above its m. p., the imide loses H2O, forming 85% of [α,β-diphenylacrylenel]-2, I-benzimidazole (I), brown, m. 186°. The concentrated H2SO4 solution is brownish red with a violet tinge. I also results by heating the components but in very poor yields. I, heated with KOH in EtOH and then acidified with AcOH, yields β-[benzimidazolyl-2'']-α,β-diphenylacrylic acid (II), contains 1 H2O, gradually turns orange on heating and m. 186° (decomposition). After standing several days in absolute EtOH, it contains 1 mol. EtOH. Et ester, short needles, which yield I on heating. Anilide, m. 278° (decomposition). The condensation of o-C6H4(NH2)2 and homophthalic anhydride in boiling EtOH yields 2-[carboxymethyl]-benz-[2'-aminoanilide], o-HO2CCH2C6H4CONHC6H4NH2(?), turns yellow at 150° and then gradually m. Ag salt, sensitive to light. o-Phenyleneacetyl-2,I-benzimidazole (III), yellow, m. 345° (decomposition), results upon heating the base at 200° for 10 min. It is not affected by MeONa in MeOH, concentrated NH4OH at 100 or 200°, PhNH2 at 190° or boiling PhNH2-Diphenic anhydride and o-C6H4(NH2)2 give a 71% yield of diphen-2''-aminoanilidecarboxylic acid, o-HO2CC6H4C6H4CONHC6H4NH2, starts to decompose 123°. From EtOH it seps. with 1 mol. of EtOH of crystallization Heated at 150°, H2O is evolved and a 70% yield of 2',I-[o-benzoylene]-2-phenylbenzimidazole (IV), m. 177-8° results, also formed in about the same yield by heating the components at 150°. Unlike the 6-membered ring of III, this compound yields 2'-[benzimidazolyl-2'']-diphenyl-2-carboxylic acid, m. 206-9°. Ag salt. Et ester, m. 143° (decomposition). Amide, decomps. 227°. Anilide, decomps. 248°. N-β-Phenylhydrazide, decomps. 157°. A by-product in the production of IV is N-[2''-acetaminophenyl]diphenimide, decomps. 233°, which also results by

heating the anilide with AcCl. It is probably (C6H4CO)2NC6H4NHAc.

IT 861783-93-9P, 2-Benzimidazoleacrylanilide, α,β-diphenyl-
RL: PREP (Preparation)
(preparation of)

RN 861783-93-9 CAPLUS

CN Benzeneacetamide, α-(1H-benzimidazol-2-ylphenylmethylene)-N-phenyl-
(CA INDEX NAME)



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